

The Inducibility of Graphs on Four Vertices

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Abstract

We consider the problem of determining the maximum induced density of a graph H in any graph on n vertices. The limit of this density as n tends to infinity is called the inducibility of H . The exact value of this quantity is known only for a handful of small graphs and a specific set of complete multipartite graphs. Answering questions of [2] and [3] we determine the inducibility of $K_{1,1,2}$ and the paw graph. The proof is obtained using semi-definite programming techniques based on a modern language of extremal graph theory, which we develop in full detail in an accessible setting.

1 Introduction

Following the notation of [3], for graphs H, G with $|V(H)| = k$, $|V(G)| = n$ we define $I(H; G)$ as the number of induced subgraphs of G isomorphic to H . Since we are not concerned with the size of G , we normalize $I(H; G)$ in a suitable way by defining $i(H; G) = I(H; G) / \binom{n}{k}$. We are now able to define the *inducibility* of a graph H as

$$i(H) = \lim_{n \rightarrow \infty} \max_{\substack{G \\ |V(G)|=n}} i(H; G).$$

It is not difficult to see that this limit always exists. The problem of determining $i(H)$ appears to be non-trivial even in some cases when H is a very small graph. Let \overline{H} denote the complement graph of H . Note that we have that $i(H) = i(\overline{H})$, so that we need only consider one graph in a complementary pair. The inducibility of all graphs on less than four vertices is known. There are 11 non-isomorphic graphs on four vertices: five complementary pairs and one self-complementary graph. The case of K_4 , the complete graph on four vertices is trivial, as for any complete graph K_n we have $i(K_n) = i(\overline{K_n}) = 1$.

In [3], Exoo gave upper and lower bounds on $i(H)$ for the remaining 4-vertex graphs. Since then the inducibility of some of these graphs has been determined. In [1], Bollobás *et al.* studied the inducibility of balanced complete bipartite graphs $K_{r,r}$, and proved that the graph which maximizes $i(K_{r,r}; G)$ is again a balanced complete bipartite graph $K_{n,n}$. This resolved the case of $K_{2,2}$ and its complement. Later in [2], Brown and Sidorenko proved that if H is a complete bipartite graph, then the graph which maximizes $i(H; G)$ can also be chosen to be complete bipartite, resolving $K_{1,3}$ and its complement. They also gave a generalization to complete multi-partite graphs, along with conditions under which the exact graph G is known. However, the inducibility of the complete tri-partite $K_{1,1,2}$ is not classified by these conditions.

There remain three 4-vertex graphs (considering one from each complementary pair) for which the exact value of $i(H)$ is unresolved: $K_{1,1,2}$, the paw graph (the graph obtained from a triangle by adding a pendant edge) H_{paw} , and the path on four vertices P_4 . Brown and Sidorenko mentioned

in [2] that the best construction they know for $K_{1,1,2}$ is a balanced complete multipartite graph with 5 parts (a “5-equipartite graph” by their convention). Making use of the recent theory of flag algebras from [14] and semi-definite programming techniques used in [15, 10, 6, 8, 7] among other papers, we determine $i(K_{1,1,2})$, and $i(H_{\text{paw}})$, and show that the construction of Brown and Sidorenko is in fact best possible.

A detailed account of the semi-definite method in extremal graph theory is not easily accessible. The description given in [14] is difficult, as it is presented in a very general language, and other accounts are often given in terms of hypergraphs, so we will give a full development of the methods by which we obtained our results. Our notation differs slightly from that of the flag algebras introduced by Razborov in [14], so we present in the next section the basic definitions which will be needed. Following this, we present the semi-definite program which does the bulk work in obtaining our results, and show how to interpret the output of the solver. Finally, we give techniques, some known and some new, for obtaining the best possible proof.

2 Preliminaries

2.1 Homomorphism Densities

For two graphs H and G , a graph *homomorphism* from H to G is a map $\varphi : V(H) \rightarrow V(G)$ which preserves adjacency, i.e. φ is such that $(u, v) \in E(H) \implies (\varphi(u), \varphi(v)) \in E(G)$ for every $u, v \in V(H)$. Now we can define $t(H; G)$ as the probability that a uniformly chosen map $\varphi : V(H) \rightarrow V(G)$ is a homomorphism. The quantity $t(H; G)$ is called the homomorphism density of H in G . We similarly define $t_{\text{ind}}(H; G)$ with the additional condition that the homomorphisms should also preserve non-adjacency.

While $t(H; G)$ is interesting in its own right, extremal graph theory more often studies the quantity $t^{\text{inj}}(H; G)$, which is defined as the probability that a uniformly chosen *injective* map φ is a homomorphism. However, the following lemma due to Lovász and Szegedy in [12] shows that the two are close up to an error term of $o(1)$.

Lemma 2.1. *For every two graphs H , and G ,*

$$|t(H; G) - t^{\text{inj}}(H; G)| \leq \frac{1}{|V(G)|} \binom{|V(H)|}{2} = o_{|V(G)| \rightarrow \infty}(1).$$

For our purposes, Lemma 2.1 will allow us to restrict our attention to the more nicely behaved function $t(H; \cdot)$. Now we give an alternative, but useful definition of $t(H; G)$ and $t_{\text{ind}}(H; G)$ in terms of A_G , the adjacency matrix of G . For graphs H and G , let $\{x_u \mid u \in V(H)\}$ be random variables which take values from $V(G)$ uniformly. Then we have

$$t(H; G) = \mathbb{E} \left[\prod_{(u,v) \in E(H)} A_G(x_u, x_v) \right], \quad (1)$$

and

$$t_{\text{ind}}(H; G) = \mathbb{E} \left[\prod_{(u,v) \in E(H)} A_G(u, v) \prod_{(u,v) \notin E(H)} (1 - A_G(x_u, x_v)) \right]. \quad (2)$$

The two functions are related by

$$t(H; \cdot) = \sum_{\substack{F \supseteq H \\ V(F) = V(H)}} t_{\text{ind}}(F; \cdot), \quad (3)$$

and a Möbius inversion formula

$$t_{\text{ind}}(H; \cdot) = \sum_{\substack{F \supseteq H \\ V(F) = V(H)}} (-1)^{|E(F) \setminus E(H)|} t(F; \cdot). \quad (4)$$

2.2 Graphons

A sequence of graphs $\{G_i\}_{i=1}^\infty$ is called *convergent* if, for every graph H , the sequence $\{t(H; G_i)\}_{i=1}^\infty$ converges. It is not difficult to construct convergent sequences $\{G_i\}_{i=1}^\infty$ such that their limits cannot be recognized as graphs, i.e. there is no graph G with $\lim_{i \rightarrow \infty} t(H; G_i) = t(H; G)$ for every H . For this reason, the extremal solution to a problem is often stated as a sequence of graphs rather than a single graph. However, there is a “soft analytic” approach which enables us to avoid working with sequences. We can extend the space of graphs, and represent the limits of convergent sequences of graphs as an object in this extended space. It is shown in [12] that the limit of a convergent graph sequence can be represented as a measurable, symmetric function $w : [0, 1]^2 \rightarrow [0, 1]$. Let \mathcal{W} denote the set of all such functions. The elements of \mathcal{W} are called *graphons*. We can extend the definition of the functions $t(H; \cdot)$ and $t_{\text{ind}}(H; \cdot)$ to graphons. Let $\{x_u \mid u \in V(H)\}$ be independent random variables which take values uniformly from $[0, 1]$. Then for $w \in \mathcal{W}$, we define

$$t(H; w) = \mathbb{E} \left[\prod_{(u,v) \in E(H)} w(x_u, x_v) \right], \quad (5)$$

and

$$t_{\text{ind}}(H; w) = \mathbb{E} \left[\prod_{(u,v) \in E(H)} w(x_u, x_v) \prod_{(u,v) \notin E(H)} (1 - w(x_u, x_v)) \right]. \quad (6)$$

Let G be a graph with $|V(G)| = n$, and define a graphon w_G as follows. Let $w_G(x, y) = A_G(\lceil xn \rceil, \lceil yn \rceil)$ for $(x, y) \in (0, 1]^2$, and $w_G = 0$ otherwise. Comparing (1) and (5), it is easy to see that we have $t(H; G) = t(H; w_G)$ (and $t_{\text{ind}}(H; G) = t_{\text{ind}}(H; w_G)$ similarly) for every H, G . In this sense graphons are a natural extension of finite graphs. Furthering this notion, Lovász and Szegedy show in [12] that the space of graphons \mathcal{W} is complete in the sense that every convergent sequence of graphons converges to a graphon, and also that the set $\{w_G \mid G \text{ is a finite graph}\}$ is dense in \mathcal{W} . That is, if $\{w_i\}_{i \in \mathbb{N}}$ is a convergent sequence of graphons, then there exists a graphon w such that $\lim_{i \rightarrow \infty} t(H; w_i) = t(H; w)$ for every finite graph H , and furthermore for every graphon w , there exists a sequence of finite graphs $\{G_i\}_{i \in \mathbb{N}}$ such that $\lim_{i \rightarrow \infty} t(H; w_{G_i}) = t(H; w)$ for every graph H .

Graphons allow us to give a simpler analogue of $i(H)$ in the language of homomorphisms. For a graph H , let $\Gamma(H)$ denote its group of automorphisms. Then we define

$$t_{\text{ind}}(H) = \max_{w \in \mathcal{W}} t_{\text{ind}}(H; w) = \frac{|\Gamma(H)|}{|V(H)|!} i(H). \quad (7)$$

Note that the fact that the maximum in (7) is attained follows from the completeness of the space of graphons and the compactness of $[0, 1]^{\mathbb{N}}$.

2.3 Quantum Graphs

A *k-partially labeled graph* is a graph in which k of the vertices have been labeled with distinct natural numbers $1, \dots, k$. We extend the definition of $t(\cdot; w)$ for partially labeled graphs. For a

k -partially labeled graph H , and a map $\phi : [k] \rightarrow [0, 1]$, we define $t(H, \phi; w)$ as $t(H; w)$ in (5), conditioned on the event that $x_i = \phi(i)$, $1 \leq i \leq k$.

The function $\llbracket \cdot \rrbracket$ maps k -partially labeled graphs to graphs by unlabeled the labeled vertices. This function can be seen as an averaging map, as for a k -partially labeled graph H , we have

$$t(\llbracket H \rrbracket; w) = \mathbb{E}_{\phi} t(H, \phi; w), \quad (8)$$

where $\phi : [k] \rightarrow [0, 1]$ is a uniformly chosen map. We define the product of k -partially labeled graphs H_1 and H_2 , denoted $H_1 \cdot H_2$, by taking the disjoint union of H_1 and H_2 as graphs and then identifying the labeled vertices, reducing multiple edges. Note that by this definition we have the property that

$$t(F \cdot G, \phi; w) = t(F, \phi; w)t(G, \phi; w), \quad (9)$$

for k -partially labeled graphs F, G and any compatible map ϕ .

Let \mathcal{F}_k denote the set of all k -partially labeled graphs. Together with the above product, \mathcal{F}_k has the structure of a commutative semigroup. Now let $\mathbb{R}[\mathcal{F}_k]$ denote the semigroup algebra of \mathcal{F}_k over \mathbb{R} . That is, elements of $\mathbb{R}[\mathcal{F}_k]$ are formal finite linear combinations of elements of \mathcal{F}_k , and the product on $\mathbb{R}[\mathcal{F}_k]$ is obtained from the product on \mathcal{F}_k by distributivity over addition. Elements of $\mathbb{R}[\mathcal{F}_k]$ are called *k-quantum graphs* (we will refer to 0-quantum graphs as simply quantum graphs). We extend the definition of the functions $t(\cdot, \phi; w)$ and $\llbracket \cdot \rrbracket$ to k -quantum graphs in the natural way (by linearity). It follows from (9) that for every fixed graphon w and map $\phi : [k] \rightarrow [0, 1]$, the function $t(\cdot, \phi; w) : \mathbb{R}[\mathcal{F}_k] \rightarrow \mathbb{R}$ is an algebra homomorphism. Let \mathcal{K}_k denote the intersection of the kernels of all these algebra homomorphisms. In other words,

$$\mathcal{K}_k = \{f \in \mathbb{R}[\mathcal{F}_k] \mid t(f, \phi; w) = 0 \quad \forall \phi, w\}.$$

Then \mathcal{K}_k is a subalgebra and we obtain the quotient algebra \mathcal{A}^k by $\mathcal{A}^k = \mathbb{R}[\mathcal{F}_k]/\mathcal{K}_k$. For k -quantum graphs f and g , we will make use of the notation $f = g$, which should be taken in the sense that f and g are equal in \mathcal{A}^k , that is $f - g \in \mathcal{K}_k$. Note that for every k -partially labeled graph H , we have

$$H = H \cup K_1. \quad (10)$$

For a k -partially labeled graph H , the k -quantum graph $\text{Ind}(H)$ is defined as

$$\sum_{\substack{F \supseteq H \\ V(F)=V(H)}} (-1)^{|E(F) \setminus E(H)|} F.$$

Note that it follows from (4) that $t_{\text{ind}}(H, \phi; w) = t(\text{Ind}(H), \phi; w)$ for every ϕ, w .

A partially labeled graph in which all the vertices are labeled is called a *type*. For a fixed type σ , let H be a partially labeled graph for which the labeled vertices induce a subgraph isomorphic (by a label preserving isomorphism) to σ . Then $\text{Ind}(H) \in \mathcal{A}^k$ is called a σ -flag. Let $\text{Ind}(F), \text{Ind}(H)$ be σ_1, σ_2 -flags, respectively, with $\sigma_1 \neq \sigma_2$. Then $\text{Ind}(F) \cdot \text{Ind}(H) = 0$, since for any ϕ, w , at least one of $t(\text{Ind}(F), \phi; w)$, $t(\text{Ind}(H), \phi; w)$ is zero.

For every type σ on $k \geq 1$ vertices, let \mathcal{A}^σ be the subalgebra of \mathcal{A}^k spanned by the set $\{f \in \mathcal{A}^k \mid f \text{ is a } \sigma\text{-flag}\}$. If $\sigma_1, \dots, \sigma_r$ are all the non-isomorphic types on k vertices, then we have the orthogonal decomposition $\mathcal{A}^k = \bigoplus_{i=1}^r \mathcal{A}^{\sigma_i}$. In other words, for every $f \in \mathcal{A}^{\sigma_i}$ and $g \in \mathcal{A}^{\sigma_j}$ with $i \neq j$, we have $f \cdot g = 0$.

Remark 2.2. The reader should be warned that our notation here slightly differs from that of Razborov in [14]. A σ -flag H in Razborov's language corresponds to $(u!/|\Gamma(H)|)\text{Ind}(H)$ in our language, where u is the number of unlabeled vertices in H , and $\Gamma(H)$ refers here to the group of label preserving automorphisms of H . We believe that our notation has the advantage that the product of the algebra A^σ , and the operator $\llbracket \cdot \rrbracket$ have easier descriptions.

The crux of our results rely on the following easy lemma.

Lemma 2.3. *Let f be a k -quantum graph, then*

$$t(\llbracket f^2 \rrbracket; w) \geq 0$$

for all graphons w .

Proof. Fix a map $\phi : [k] \rightarrow [0, 1]$, and let $f = \sum_{i=1}^n \alpha_i H_i$. Then we have

$$\begin{aligned} t(f^2, \phi; w) &= t\left(\left(\sum_{i=1}^n \alpha_i H_i\right)^2, \phi; w\right) = t\left(\sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j H_i \cdot H_j, \phi; w\right) \\ &= \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j t(H_i, \phi; w) t(H_j, \phi; w) = \left(\sum_{i=1}^n \alpha_i t(H_i, \phi; w)\right)^2 \geq 0. \end{aligned}$$

Now our desired result follows from (8), which shows that the function $\llbracket \cdot \rrbracket$ preserves positivity. \square

Remark 2.4. It follows from Lemma 2.3 that for any k -quantum graphs f_1, \dots, f_n , and any graphon w , the $n \times n$ matrix \mathbf{M} defined by $\mathbf{M}(i, j) = t(\llbracket f_i \cdot f_j \rrbracket; w)$ is positive semi-definite (PSD). To see this, note that we can write

$$z^T M z = \sum_{i,j} z_i z_j t(\llbracket f_i \cdot f_j \rrbracket; w) = t\left(\left\llbracket \left(\sum_i z_i f_i\right)^2 \right\rrbracket; w\right) \geq 0.$$

This is the basis for the so called semi-definite method in extremal graph theory.

3 The Semi-Definite Method

3.1 The Semi-Definite Program and its Dual

It follows from reflection positivity characterizations [4, 12, 13] that every asymptotic algebraic inequality between subgraph densities follows from the positive semi-definiteness of a certain infinite matrix. If this matrix were finite, then it would be possible to solve every such inequality efficiently using semi-definite programming. However, since the matrix is infinite, in practice one can only consider a finite sub-matrix and hope that the inequality still holds under the weaker condition that the sub-matrix is positive semi-definite. We call this approach the semi-definite method in extremal graph theory. First let us recall the standard form of a semi-definite program (SDP) and its dual.

The primal SDP formulation we will make use of is the following

$$\begin{aligned} &\text{minimize} && c \cdot x \\ &\text{subject to} && \mathbf{X} = \sum_{i=1}^m \mathbf{F}_i x_i - \mathbf{F}_0 \succeq 0 \end{aligned} \tag{11}$$

and the corresponding dual program is

$$\begin{aligned} & \text{maximize} && \mathbf{F}_0 \bullet \mathbf{Y} \\ & \text{subject to} && \mathbf{F}_i \bullet \mathbf{Y} = c_i \quad 1 \leq i \leq m, \quad \mathbf{Y} \succeq 0 \end{aligned} \tag{12}$$

where $c \in \mathbb{R}^m$, $\mathbf{F}_i \in \mathbb{R}^{n \times n}$ are given, and $x \in \mathbb{R}^m$, $\mathbf{Y} \in \mathbb{R}^{n \times n}$ are variables. Note that $c \cdot x$ refers to the standard dot product, while $\mathbf{F}_0 \bullet \mathbf{Y}$ refers to the inner product on $\mathbb{R}^{n \times n}$ defined by $A \bullet B = \text{Tr}(A^T B) = \sum_{i,j} A_{i,j} B_{i,j}$. The duality here refers to the fact (see e.g. [11]) that if (11) is feasible, then its solution is equal to the solution to (12).

Now fix a quantum graph $f = \sum_{i=1}^m \alpha_i H_i$, and suppose we want to find

$$\min_{w \in \mathcal{W}} t(f; w). \tag{13}$$

Many statements in asymptotic extremal graph theory can be converted to this form. For example, the celebrated Goodman bound [5] says that $\min_{w \in \mathcal{W}} t(K_3 - 2(K_2 \cup K_2) + K_2; w) \geq 0$.

Choose two parameters $0 \leq L \leq N$, where N is large enough so that

$$f \in \text{Span}\{H : H \text{ is an } N\text{-vertex graph}\} \subseteq \mathcal{A}^0.$$

For every $1 \leq k \leq L$, let $\{f_1^k, \dots, f_{m_k}^k\}$ be a set of independent k -quantum graphs on $\lfloor (N+k)/2 \rfloor$ vertices, so that by (10) we have

$$f_i^k \cdot f_j^k \in \text{Span}\{H : H \text{ is an } N\text{-vertex } k\text{-partially labeled graph}\} \subseteq \mathcal{A}^k.$$

By (10), we can assume that H_1, \dots, H_m in (13) are all the non-isomorphic graphs on N vertices. Consider the following semi-definite program:

$$\begin{aligned} & \text{minimize} && \sum_{i=1}^m \alpha_i x_{H_i} \\ & \text{subject to} && x_{K_1} = 1; \\ & && \forall k \leq L, \text{ the matrix } \mathbf{M} \text{ defined by } \mathbf{M}(u, v) = \sum_{i=1}^m \beta_i x_{H_i} \text{ is PSD,} \\ & && \text{where } \sum_{i=1}^m \beta_i H_i := \llbracket f_u^k \cdot f_v^k \rrbracket. \end{aligned} \tag{14}$$

One should interpret the values x_H in (14) as $t(H; w)$, for some w . Note then that Remark 2.4 shows that these semi-definiteness constraints are in fact necessary. By this interpretation, the solution to (14) will be a lower bound for (13). By choosing L and N large enough, this lower bound will often be quite good, and in some cases best possible. This is not the case for any choice of f , however. In [9], it is shown that there exists quantum graphs f for which no choice of L and N will give a sharp bound. In fact, they show that determining the value of (13) for general quantum graphs f is undecidable.

It is not too hard to see how to convert (14) to the form (11). To implement the constraints as a semi-definiteness condition, we make use of the fact that a block diagonal matrix is PSD if and only if all of its diagonal blocks are. Each constraint is implemented using one block. For the first L blocks, the uv -th entry in the k -th block of \mathbf{F}_{i_0} is given by β_{i_0} , where $\llbracket f_u^k \cdot f_v^k \rrbracket = \sum_{i=1}^m \beta_i H_i$. We use the last block (i.e. the $(L+1)$ -th block) to implement the first constraint. We want $x_{K_1} - 1 \geq 0$ and $1 - x_{K_1} \geq 0$, which are implemented making use of the constant matrix \mathbf{F}_0 .

3.2 Extracting an Upper Bound

Suppose the optimal solution to (14) is α . Then our above discussion shows that α is a lower bound for $t(f, w)$. In Section 3.1, we saw how (14) can be converted to the form (11). By duality, the

optimal solution to the dual problem (12) is also α . The matrix \mathbf{Y} from the dual problem encodes a proof of this, which we can extract. The constraint on $\mathbf{Y} \succeq 0$ is that $\mathbf{F}_i \bullet \mathbf{Y} = \alpha_i$. So we have

$$\sum_{i=1}^m (\mathbf{F}_i \bullet \mathbf{Y}) H_i = \sum_{i=1}^m \alpha_i H_i = f.$$

For every $1 \leq k \leq L$, let $\mathbf{Y}^{(k)}$ denote the k -th block of \mathbf{Y} . That is the block that corresponds to the positive semi-definiteness constraint created by $\{f_1^k, \dots, f_{m_k}^k\}$ in (14). Similarly let $\mathbf{F}_i^{(k)}$ denote the k -th block of \mathbf{F}_i for every $1 \leq i \leq m$ and every $1 \leq k \leq L$.

By splitting the inner product between the last block (the $x_{K_1} = 1$ constraint) and the rest of the blocks, it follows from $\mathbf{F}_0 \bullet \mathbf{Y} = \alpha$ that

$$\sum_{i=1}^m \sum_{k=1}^L \left(\sum_{u=1}^{m_k} \sum_{v=1}^{m_k} \mathbf{F}_i^{(k)}(u, v) \mathbf{Y}^{(k)}(u, v) \right) H_i = f - \alpha K_1 = f - \alpha.$$

Here we use α to denote the quantum graph αK_1 as a slight abuse of notation, based on the fact that $t(\alpha K_1; w) = \alpha$ for all graphons w . Exchanging the order of summation, and using the definition of \mathbf{F}_ℓ , this reduces to

$$f - \alpha = \sum_{k=1}^L \sum_{u=1}^{m_k} \sum_{v=1}^{m_k} \mathbf{Y}^{(k)}(u, v) \llbracket f_u^k \cdot f_v^k \rrbracket = \sum_{k=1}^L \llbracket z_k^T \mathbf{Y}^{(k)} z_k \rrbracket,$$

where z_k is the vector $(f_1^k, \dots, f_{m_k}^k)^T$.

Remark 3.1. For any matrix $A \succeq 0$ and vector of k -quantum graphs z , the quantum graph $\llbracket z^T A z \rrbracket$ is trivially positive. To see this, notice that for any map $\phi : [k] \rightarrow [0, 1]$ and a graphon w , we can write

$$t(z^T A z, \phi; w) = \sum_{i,j} A(i, j) t(z_i, \phi; w) t(z_j, \phi; w) = v^T A v \geq 0,$$

where v is defined by $v_i = t(z_i, \phi; w)$. Now the positivity of $\llbracket z^T A z \rrbracket$ follows as in Lemma 2.3.

In particular, Remark 3.1 shows that the quantum graph $f - \alpha$ is positive, i.e. $t(f; w) \geq \alpha$ for every graphon w .

Remark 3.2. Since \mathbf{Y} is positive semi-definite, every block $\mathbf{Y}^{(k)}$ is also positive semi-definite. Performing an eigenvalue decomposition on each $\mathbf{Y}^{(k)}$, and noting that $\mathbf{Y}^{(k)} \succeq 0$ has non-negative eigenvalues, we can get the useful form

$$f - \alpha = \sum_{i=1}^r \lambda_i \llbracket g_i^2 \rrbracket,$$

where each $g_i \in \text{Span}(\{f_1^k, \dots, f_{m_k}^k\})$, for some k .

3.3 Some Remarks

From Remark 3.2, we can see that the choice of sets $\{f_1^k, \dots, f_{m_k}^k\}$ is key in obtaining a proof of our desired bound. To have the best chance of finding a proof, we should choose $f_1^k, \dots, f_{m_k}^k$ so that they span the entire algebra \mathcal{A}^k . One simple choice is to use the set of all k -partially labeled graphs on $\lfloor (N + k)/2 \rfloor$ vertices. However, the resulting matrix \mathbf{Y} will be dense, and it is in our interests to obtain as small and simple a proof as possible. As a first measure, note that the size of

\mathbf{Y} increases exponentially with the parameters L and N , so we should choose these to be minimal while still getting the desired bound.

The set

$$\{\text{Ind}(F) : F \text{ is a } \lfloor (N+k)/2 \rfloor\text{-vertex } k\text{-partially labeled graph}\}$$

makes a particularly good basis for \mathcal{A}^k . It follows easily from (3) and (4) that this is indeed a basis for \mathcal{A}^k . We can partition this set according to the type obtained by restricting each F to its labeled vertices. Then the partition corresponding to each type σ is a basis for \mathcal{A}^σ . Because of the orthogonality properties these subspaces enjoy, by this choice of basis each diagonal block of the matrix \mathbf{Y} reduces to a number of smaller blocks: one for each type on k vertices.

We should also note here that not even all these blocks are required. If $\sigma_1 \neq \sigma_2$ are two types such that $\llbracket \sigma_1 \rrbracket = \llbracket \sigma_2 \rrbracket$, then for every $g \in \mathcal{A}^{\sigma_1}$, there exists some $f \in \mathcal{A}^{\sigma_2}$ such that $\llbracket g \rrbracket = \llbracket f \rrbracket$. Thus we only need a block for each type taken up to (not necessarily label preserving) isomorphism.

The structure of \mathcal{A}^σ is studied in detail in [14], and it provides a decomposition of \mathcal{A}^σ as a direct sum of two smaller algebras. The group $\Gamma(\llbracket \sigma \rrbracket)$ acts on \mathcal{A}^σ by permuting the labels. Then it can be shown that we can decompose \mathcal{A}^σ orthogonally as $\mathcal{A}^{\sigma,+} \oplus \mathcal{A}^{\sigma,-}$ (the “invariant” and “anti-invariant” parts) where

$$\mathcal{A}^{\sigma,+} = \{f \in \mathcal{A}^\sigma \mid \pi(f) = f \quad \forall \pi \in \Gamma(\llbracket \sigma \rrbracket)\},$$

and

$$\mathcal{A}^{\sigma,-} = \{f \in \mathcal{A}^\sigma \mid \sum_{\pi \in \Gamma(\llbracket \sigma \rrbracket)} \pi(f) = 0\},$$

so that if $f \in \mathcal{A}^{\sigma,+}$, and $g \in \mathcal{A}^{\sigma,-}$, then $f \cdot g = 0$. So for each σ , choose a basis for \mathcal{A}^σ according to this decomposition, i.e. as the union of a basis for $\mathcal{A}^{\sigma,+}$ and a basis for $\mathcal{A}^{\sigma,-}$. Then each block of \mathbf{Y} further reduces to two smaller blocks.

If we have a set \mathcal{W}_0 of “conjectured extremal graphons”, i.e. graphons such that $t(f, w_0) = \alpha$, then we can also make use of the following. Let $w_0 \in \mathcal{W}_0$. Then if

$$\sum_{i=1}^r \llbracket g_i^2 \rrbracket = f - \alpha,$$

it follows that

$$\sum_{i=1}^r t(\llbracket g_i^2 \rrbracket, w_0) = 0.$$

Thus for all $1 \leq i \leq r$, we must have

$$\mathbb{E}_\phi t(g_i, \phi; w_0)^2 = \mathbb{E}_\phi t(g_i^2, \phi; w_0) = t(\llbracket g_i^2 \rrbracket; w_0) = 0,$$

which shows that $\mathbb{E}_\phi |t(g_i, \phi; w_0)| = 0$. Define $\Delta^\sigma = \{f \in \mathcal{A}^\sigma \mid \mathbb{E}_\phi |t(f, \phi; w_0)| = 0 \quad \forall w_0 \in \mathcal{W}_0\}$. Then we can reduce the size of each block of \mathbf{Y} by restricting ourselves to a basis of $\mathcal{A}^\sigma \cap \Delta^\sigma = (\Delta^\sigma \cap \mathcal{A}^{\sigma,+}) \oplus (\Delta^\sigma \cap \mathcal{A}^{\sigma,-})$.

A final remark is in regards to the floating point nature of the SDP solver. The matrix \mathbf{Y} output by the SDP corresponds to a proof of the desired bound only to a specified degree of floating point error. While some of the entries may have obvious rational closed forms (computer algebra systems are quite good at finding these), it is likely that the solver will have more degrees of freedom than required. Thus the entries will often be somewhat arbitrary floating point numbers. To resolve this, we can first attempt to restrict our bases even further. There is no obvious way to do this, and the best results will come from repeated experiments. Once we have a minimal size proof, to

resolve any remaining slackness in the solver, we can introduce further constraints to fix certain values of \mathbf{Y} to close rational approximations. By fixing only a few values, the remaining entries will often be uniquely determined rational numbers, and the solver does most of the work here.

4 Results

4.1 Representing Graphs

Before we give our results, we will need a notation that is able to concisely express a large number of partially labeled graphs. We will use an adjacency list, slightly modified for partially labeled graphs. Labeled vertices are identified by their labels, and other vertices are identified with a character. As an example, $\{1a, 1b, 2a, 2b, ab\}_{4,2}$ refers to a 4-vertex, 2-partially labeled graph (indicated in the trailing subscript) with five edges, and each pair corresponds to an edge.

4.2 A Proof of the Paw Graph

Theorem 4.1. *Let H_{paw} denote the four vertex graph obtained from a triangle by adding a single edge. Then we have*

$$t_{\text{ind}}(H_{\text{paw}}) = \frac{1}{32}.$$

Proof. We first give a graphon w_0 which achieves our desired lower bound. Let $w_0 = 1 - w_{K_2 \cup K_2}$. A simple counting argument now shows $t_{\text{ind}}(H_{\text{paw}}; w_0) = 1/32$, giving the lower bound $t_{\text{ind}}(H_{\text{paw}}) \geq 1/32$.

To prove the upper bound, we must show that $t(\text{Ind}(H_{\text{paw}}); w) \leq 1/32$ for all graphons w . Then we need to give positive semi-definite matrices \mathbf{Y}_i , and vectors of k_i -quantum graphs z_i such that $\sum [z_i^T \mathbf{Y}_i z_i] = 1/32 - \text{Ind}(H_{\text{paw}})$. In fact if H_1, \dots, H_m are all graphs on 5 vertices and $1/32 - \text{Ind}(H_{\text{paw}}) = \sum_{i=1}^m \alpha_i H_i$, then it suffices to have $\sum [z_i^T \mathbf{Y}_i z_i] = \sum_{i=1}^m \beta_i H_i$, where $\beta_i \leq \alpha_i$ for every $1 \leq i \leq m$.

Define the positive semi-definite matrices $\mathbf{Y}_1, \dots, \mathbf{Y}_6$ as

$$\begin{aligned} \mathbf{Y}_1 &= \frac{1}{96} \begin{pmatrix} 4 & -7 & -2 & -5 & 4 \\ -7 & 59 & -38 & 33 & -7 \\ -2 & -38 & 44 & -18 & -2 \\ -5 & 33 & -18 & 19 & -5 \\ 4 & -7 & -2 & -5 & 4 \end{pmatrix}, \quad \mathbf{Y}_2 = \frac{1}{1920} \begin{pmatrix} 80 & -275 & -70 \\ -275 & 1632 & -446 \\ -70 & -446 & 748 \end{pmatrix}, \\ \mathbf{Y}_3 &= \frac{1}{192} \begin{pmatrix} 32 & -43 \\ -43 & 58 \end{pmatrix}, \quad \mathbf{Y}_4 = \frac{1}{960} \begin{pmatrix} 65 & -214 \\ -214 & 839 \end{pmatrix}, \\ \mathbf{Y}_5 &= \frac{1}{12} \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}, \quad \mathbf{Y}_6 = \frac{1}{120} \begin{pmatrix} 24 & -13 \\ -13 & 10 \end{pmatrix}, \end{aligned}$$

and the vectors z_1, \dots, z_6 by

$$\begin{aligned} z_1^T &= \text{Ind}(\{ \}_{3,1}, \{1b\}_{3,1}, \{1b, ab\}_{3,1}, \{1a, 1b\}_{3,1}, \{1a, 1b, ab\}_{3,1}), \\ z_2^T &= \text{Ind}(\{3a\}_{4,3} + \{2a\}_{4,3}, \{2a, 3a\}_{4,3}, \{1a, 2a\}_{4,3}), \\ z_3^T &= \text{Ind}(\{23\}_{4,3}, \{23, 2a, 3a\}_{4,3} - \{1a, 23\}_{4,3} - \{1a, 23, 3a\}_{4,3}), \\ z_4^T &= \text{Ind}(\{23, 3a\}_{4,3} - \{23, 2a\}_{4,3}, \{1a, 23, 3a\}_{4,3} - \{1a, 23, 2a\}_{4,3}), \end{aligned}$$

$$z_5^T = \text{Ind}(\{13, 23\}_{4,3} - \{13, 23, 2a\}_{4,3}, \{13, 1a, 23, 2a\}_{4,3} - \{13, 1a, 23, 2a, 3a\}_{4,3}),$$

$$z_6^T = \text{Ind}(\{13, 23, 2a\}_{4,3}, \{13, 23, 2a, 3a\}_{4,3} - \{13, 1a, 23, 3a\}_{4,3}),$$

where as a slight abuse of notation, $\text{Ind}(\cdot)$ applied to a row vector is defined by applying $\text{Ind}(\cdot)$ to all its entries. It can be verified that \mathbf{Y}_i , and z_i satisfy the conditions given above, so the desired upper bound holds, and the result follows. \square

4.3 A Proof of $K_{1,1,2}$

Theorem 4.2. *We have*

$$t_{\text{ind}}(K_{1,1,2}) = \frac{12}{125} = 0.096.$$

Proof. The construction given by Brown and Sidorenko in [2] corresponds to the graphon w_{K_5} , and a simple counting argument gives $t_{\text{ind}}(K_{1,1,2}; w_{K_5}) = 12/125$, giving us the lower bound.

The proof of the upper bound is as in the proof of Theorem 4.1, except that instead of $1/32 - \text{Ind}(H_{\text{paw}})$ we are dealing with $12/125 - \text{Ind}(K_{1,1,2})$. We must also take H_1, \dots, H_m to be all the graphs on 7 vertices. The matrices $\mathbf{Y}_1, \dots, \mathbf{Y}_6$ are defined as

$$\mathbf{Y}_1 = \frac{1}{180000} \begin{pmatrix} 17280 & -24912 & -79032 & 17916 & 27236 \\ -24912 & 70560 & 193926 & -71271 & -62329 \\ -79032 & 193926 & 587520 & -205728 & -185320 \\ 17916 & -71271 & -205728 & 113760 & 52920 \\ 27236 & -62329 & -185320 & 52920 & 62640 \end{pmatrix},$$

$$\mathbf{Y}_2 = \frac{1}{7500} \begin{pmatrix} 270 & 2991 & -90 \\ 2991 & 33150 & -997 \\ -90 & -997 & 30 \end{pmatrix},$$

$$\mathbf{Y}_3 = \frac{1}{5000} \begin{pmatrix} 3075 & 5514 & 1483 & 3917 \\ 5514 & 14500 & 8915 & 12585 \\ 1483 & 8915 & 9320 & 9490 \\ 3917 & 12585 & 9490 & 11725 \end{pmatrix}, \quad \mathbf{Y}_4 = \frac{1}{100} (23),$$

$$\mathbf{Y}_5 = \frac{1}{300000} \begin{pmatrix} 95040 & -81360 & -68250 & -225285 & 43415 \\ -81360 & 417600 & 350340 & 749826 & -222822 \\ -68250 & 350340 & 294000 & 629130 & -186960 \\ -225285 & 749826 & 629130 & 1425600 & -400105 \\ 43415 & -222822 & -186960 & -400105 & 107007 \end{pmatrix},$$

$$\mathbf{Y}_6 = \frac{1}{1200000} \begin{pmatrix} 343560 & -310680 & -234812 & 53570 \\ -310680 & 190272 & 119819 & -34343 \\ -234812 & 119819 & 75456 & -21579 \\ 53570 & -34343 & -21579 & 9910 \end{pmatrix},$$

and the vectors z_1, \dots, z_6 are given by

$$z_1^T = \text{Ind}(\{\}_{4,1}, \{1c, ac, bc\}_{4,1}, \{1b, 1c, ab, ac\}_{4,1}, \{1a, 1b, 1c\}_{4,1}, \{1a, 1b, 1c, ac, bc\}_{4,1}),$$

$$z_2^T = \text{Ind}(\{1b, 2b, ab\}_{4,2}, \{1b, 2a, ab\}_{4,2}, \{1a, 1b, 2a, 2b, ab\}_{4,2}),$$

$$z_3^T = \text{Ind}(\{12\}_{4,2}, \{12, 2b\}_{4,2} + \{12, 1b\}_{4,2}, \{12, 1b, 2b\}_{4,2}, \{12, 1b, 2a, 2b\}_{4,2} + \{12, 1a, 1b, 2b\}_{4,2}),$$

$$\begin{aligned}
z_4^T &= \text{Ind}(\{12, 2b\}_{4,2} - \{12, 1b\}_{4,2}), \\
z_5^T &= \text{Ind}(\{13, 23, 3a, 3b\}_{5,3}, \{13, 1b, 23, 2b, 3a, 3b\}_{5,3}, \{13, 1b, 23, 2a, 2b, 3a\}_{5,3} + \{13, 1a, 1b, 23, 2b, 3a\}_{5,3}, \\
&\quad \{13, 1a, 1b, 23, 2a, 2b\}_{5,3}, \{13, 1a, 1b, 23, 2a, 2b, 3a, 3b\}_{5,3}), \\
z_6^T &= \text{Ind}(\{12, 13, 1b, 23, 2a, 3a, 3b, ab\}_{5,3} + \{12, 13, 1b, 23, 2a, 2b, 3a, ab\}_{5,3} + \{12, 13, 1a, 1b, 23, 2b, 3a, ab\}_{5,3}), \\
&\quad \{12, 13, 1b, 23, 2a, 2b, 3a, 3b, ab\}_{5,3} + \{12, 13, 1a, 1b, 23, 2b, 3a, 3b, ab\}_{5,3}, \\
&\quad \{12, 13, 1a, 1b, 23, 2a, 2b, 3b, ab\}_{5,3}, \{12, 13, 1a, 1b, 23, 2a, 2b, 3a, 3b, ab\}_{5,3}).
\end{aligned}$$

□

5 Conclusion and Open Problems

The semi-definite method is a powerful technique for proving inequalities between subgraph densities, although it has its drawbacks. The proof we gave for the case of $K_{1,1,2}$ was obtained by efforts near the limit of our computing power. We had to run the semi-definite program with graphs on seven vertices (i.e. $N = 7$ in (14)). The solver took 2-3 hours to run on full precision, and the search space (and thus running time) grows exponentially with the number of vertices. Proofs by this method for larger graphs (7+ vertices) seem not to be feasible, but even some small graphs elude us. The only remaining unresolved graph on 4 vertices is the self-complementary P_4 .

The case of $t_{\text{ind}}(P_4)$ is interesting. The upper bound given by Exoo in [3] was (converting to our language) $1/36 = 0.0277$. Using the semi-definite method, we can improve this to a floating point bound of roughly 0.0172, but we conjecture that this bound is not tight either. In our experience, when the solver gives a tight bound, the value has a simple closed form, but this is not the case here. The best construction we know of for P_4 is still the one given by Exoo, involving the Paley Graph $QR(17)$. The corresponding lower bound is $80/4877 \approx 0.0164$, so there is a clear gap between this construction and the best bounds we can obtain.

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